Order parameter fluctuation effects in d-wave BCS superconductors

Hyok-Jon Kwon*
Department of Physics, University of Florida, Gainesville, FL 32611-8440
(February 1, 2008)

We study order parameter fluctuation effects in the superconducting state as a possible precursor to the pseudogap phenomena. Using a low-energy effective theory in the d-wave BCS model, we self-consistently calculate the single-particle properties. We find that the fluctuations reduce the spectral gap, and the shape of the gap is deformed, showing reduced slope of the gap at the nodes. We also show the angle-dependence of the quasiparticle lifetime due to the fluctuations.

Introduction.—Despite much experimental evidence of pseudogap phenomena in the underdoped cuprates, their microscopic mechanism is not understood.[1] However, a pairing precursor as the origin of the pseudogap is one prominent possibility.[2] An active endeavor has been to incorporate strong pairing fluctuations to account for the pseudogap phenomena, especially above the superconducting critical temperature T_c.[3,4] In this report, we take a different tack and study the order parameter fluctuation effects in the superconducting state. From a phenomenological standpoint, the pseudogap state can be considered as a superconductor whose phase coherence is destroyed by strong phase fluctuations whereas the gap is robust.[5] Therefore, it will bare similarity to a superconducting state with strong order parameter phase and amplitude fluctuations. Here we do not attempt to reproduce pseudogap phenomena since we study fluctuations in the weak-coupling BCS theory below T_c and do not consider vortex pair unbinding transition, but much of the qualitative trend is expected to pertain to the pseudogap state. Using the effective low-energy theory approach, we may describe the problem with relatively few physical parameters and separate the effect of order parameter phase and amplitude fluctuation effects.[6,7]

We address the following two issues concerning the fluctuation effects. First, we examine the effect of the order parameter fluctuations on the size of the spectral gap below T_c. It has been shown that the fluctuations reduce the magnitude of the order parameter and the critical temperature.[4,8,9] In this paper we also show the reduction in the spectral gap in a wide temperature range. For simplicity we do not the include Coulomb interaction or disorder although they would alter the form of the order parameter fluctuations and further modify our result if properly included.[4,8] Secondly, we examine the angular variation of the fluctuation effect. Angle-resolved photoemission spectroscopy (ARPES) data on underdoped cuprates show that above or below T_c the shape of the gap near the node significantly deviates from the simple d-wave shape.[10,11] We show that this may be due to the fluctuation of the phase rather than the amplitude of the order parameter, and moreover that the amplitude fluctuation effect is the strongest near the antinode. Also we discuss the angular variation of the quasiparticle lifetime.

Low-energy effective theory.—We consider the weak-coupling mean-field BCS theory in which the pairing potential gives a d-wave order parameter which is effective only within the momentum thickness $2\Lambda \ll k_F$ around the Fermi surface. Then the effective fermion Hilbert space is a thin momentum shell of a characteristic thickness 2Λ around the Fermi surface where $\Lambda \ll k_F$. For convenience, we coarse-grain the momentum shell into small boxes and label them with an angular variable ϕ. The effective action of the fermions and the order parameter is

$$S_{\rm eff} = \int d^2x \int_0^\beta d\tau \Bigg[\sum_{\phi,\sigma} c^\dagger_\sigma(\phi;\mathbf{x},\tau)\left(\partial_\tau + \frac{\nabla^2}{2m} - \mu\right) c_\sigma(\phi;\mathbf{x},\tau) + \sum_\phi \Psi^*(\mathbf{x},\tau) w(\phi) c_\downarrow(\phi;\mathbf{x},\tau) c_\uparrow(\phi+\pi;\mathbf{x},\tau) + \text{h.c.} - \frac{1}{g}\Psi^*(\mathbf{x},\tau)\Psi(\mathbf{x},\tau)\Bigg] , \quad (1)$$

where Ψ is the superconducting order parameter introduced via Hubbard-Stratonovich transformation to decouple the pairing interaction. In the above we assume a pairing potential of the form $V(\phi,\phi') = g\ w(\phi)w(\phi')$ where $w(\phi) = \cos 2\phi$ and $g < 0$ which produces a d-wave order parameter. It is understood that in writing $c_\sigma(\phi;\mathbf{k},\tau)$, the momentum $\mathbf{k}$ lives only inside the small box labeled by the angular variable ϕ near the Fermi surface. In order to explicitly separate the order parameter phase and amplitude degrees of freedom, we re-express $\Psi(\mathbf{x},\tau) = \Delta(\mathbf{x},\tau)e^{i\theta(\mathbf{x},\tau)}$ where $\Delta(\mathbf{x},\tau)$ takes a real value. In the mean-field approximation, we replace $\Delta(\mathbf{x},\tau)$ with Δ_0 and obtain a d-wave gap $\Delta(\phi) = \Delta_0 \cos 2\phi$ using the following self-consistent gap equation:

$$\frac{1}{|g|} = T\sum_\omega \sum_{\phi,\mathbf{k}} \frac{w^2(\phi)}{\omega^2 + \xi^2_{\mathbf{k}} + \Delta^2(\phi)} , \quad (2)$$

where $\xi_{\mathbf{k}} = k^2/2m - \mu$. The momentum summation above is constrained by the condition $|\xi_{\mathbf{k}}| < v_F\Lambda$. Here we consider the fluctuation around the mean-field value and re-express $\Delta(\mathbf{x},\tau) = \Delta_0 + d(\mathbf{x},\tau)$. Then we perform a gauge transformation $\psi_\sigma(\mathbf{x},\tau) = c_\sigma(\mathbf{x},\tau)e^{-i\theta(\mathbf{x},\tau)/2}$, to couple the phase fields to the fermions explicitly.

The resulting effective action is expressed in terms of the Nambu spinor notation, $\hat{\psi} = (\psi_\uparrow, \psi_\downarrow^\dagger)$, as $S_{\rm eff} = S_0 + S_I$, with

$$S_0 = T \sum_\omega \sum_{\phi,\mathbf{k}} \hat{\psi}^\dagger \hat{G}_0^{-1} \hat{\psi} \quad (3)$$
$$+ \int_0^\beta d\tau \int d^2x \Big\{ \frac{n_f}{8m} [\nabla\theta(\mathbf{x},\tau)]^2 + \frac{1}{g}[d(\mathbf{x},\tau)]^2 \Big\}$$

and

$$S_I = T \sum_\omega T \sum_\nu \sum_{\phi,\mathbf{k},\mathbf{q}} \hat{\psi}^\dagger(\phi;\mathbf{k},\omega) \Big\{ \frac{1}{2}[-\nu + i\mathbf{v}_F(\phi)\cdot\mathbf{q}]\theta(\mathbf{q},\nu)$$
$$+ w(\phi)\hat{d}(\mathbf{q},\nu) \Big\} \hat{\psi}(\phi;\mathbf{k}-\mathbf{q},\omega-\nu) \ . \quad (4)$$

Here

$$\hat{G}_0^{-1} = \begin{pmatrix} i\omega - \xi_\mathbf{k} & \Delta_0 w(\phi) \\ \Delta_0 w(\phi) & i\omega + \xi_\mathbf{k} \end{pmatrix}, \quad (5)$$

and $\hat{d}(\nu,\mathbf{q}) = \hat{\sigma}_x \ d(\nu,\mathbf{q})$, with $\hat{G}_0$ the bare Green's function for the neutral fermions. In the above, we approximate $\xi_\mathbf{k} = k^2/2m - \mu$ as $\xi_\mathbf{k} \approx v_F(|\mathbf{k}| - k_F)$ and $\mathbf{v}_F(\phi)$ is the Fermi velocity in the ϕ direction.

In building this effective theory we have not considered vortex pair unbinding which leads to the Kosterlitz-Thouless transition. This is justified well outside the fluctuation regime. We also assume that we are in the temperature range where the BCS mean-field theory is justified, namely, that $\delta T/T_c \gg \Delta_0/E_F$ in a two dimensional clean superconductor.[12] One thing we observe from the form of the effective theory is that the strength of the coupling between fermions and the amplitude fluctuations has an angle-dependence; the amplitude fluctuation effect is suppressed near the gap nodes, as is evident in Eq. (11) where the self-energy correction is multiplied by a factor of $w^2(\phi)$. The strength of the coupling to the phase fluctuations is not suppressed at the node, however.

In studying the finite temperature superconducting to normal state transition, it should be sufficient to consider only the static fluctuations of the phase, and we may suppress the time-dependence in θ and d and retain only the spatial fluctuations. Eq. (4) is then modified as

$$S_I = T \sum_\omega \sum_{\phi,\mathbf{k},\mathbf{q}} \hat{\psi}^\dagger(\phi;\mathbf{k},\omega) \Big\{ \frac{1}{2} i\mathbf{v}_F(\phi)\cdot\mathbf{q}\theta(\mathbf{q})$$
$$+ w(\phi)\hat{d}(\mathbf{q}) \Big\} \hat{\psi}(\phi;\mathbf{k}-\mathbf{q},\omega) \ . \quad (6)$$

The simplified form above, however, does not produce reliable results near zero temperature.

Fermion single-particle properties.—In evaluating the quasiparticle self-energy by perturbative expansions, we take advantage of the fact that the effective theory resides in the thin shell around the large Fermi surface and select the diagrams which are of leading order in Λ/k_F, which amounts to summing over the ring diagrams in calculating the order parameter correlation function. The fermion self-energy can be obtained self-consistently from the Dyson equation.

We first evaluate the correlation functions of the amplitude fluctuations:

$$\langle d(\mathbf{q}) \ d(-\mathbf{q})\rangle_{\rm ring} = \frac{g \ T}{1 + g\Pi_{dd}(\mathbf{q},0)} \ , \quad (7)$$

where

$$\Pi_{dd}(\mathbf{q},\nu) = \frac{1}{2} T \sum_\omega \sum_{\phi,\mathbf{k}} w^2(\phi) {\rm Tr}\Big[\hat{G}_0(\phi;\mathbf{k},\omega)\hat{\sigma}_x$$
$$\times \hat{G}_0(\phi;\mathbf{k}+\mathbf{q},\omega+\nu)\hat{\sigma}_x\Big] \ . \quad (8)$$

From Eq. (7) we obtain $\langle d(\mathbf{q}) \ d(-\mathbf{q})\rangle_{\rm ring} = T/(a + b \ q^2)$ where the temperature-dependent coefficients a and b can be evaluated by carefully expanding Π_{dd} in $\mathbf{q}$ from Eq. (8). If we only consider the spatial fluctuations in the order parameter, the $\langle d \ \theta\rangle$ terms are zero in the Gaussian approximation. Also the phase fluctuation has the following well-known correlation function[6]

$$\langle \theta(\mathbf{q})\theta(-\mathbf{q})\rangle_{\rm ring} = \frac{4mT}{n_s(T) \ q^2} \ , \quad (9)$$

where $n_s(T)$ is the superfluid density at temperature T.

Now we can determine the quasiparticle self-energy correction using the self-consistent Dyson equation, neglecting the vertex corrections:

$$\hat{\Sigma}(\phi;\mathbf{k},\omega) \approx \sum_\mathbf{q} \Big\{ \frac{1}{4} [\mathbf{v}_F(\phi)\cdot\mathbf{q}]^2 \langle\theta(\mathbf{q})\theta(-\mathbf{q})\rangle_{\rm ring} \quad (10)$$
$$+ w^2(\phi)\langle d(\mathbf{q})d(-\mathbf{q})\rangle_{\rm ring} \Big\} \hat{G}(\phi;\mathbf{k}-\mathbf{q},\omega-\nu) \ ,$$

where $\hat{G}$ is the full fermion Green's function, given self-consistently by $\hat{G}^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}$. In general the self-energy has both a momentum and frequency dependence, but we focus on the behavior of the self-energy near the Fermi surface, assuming that it varies smoothly near the Fermi surface. Therefore we neglect the $\xi_\mathbf{k}$-dependence so that the only momentum dependence is through the angle ϕ on the Fermi surface. Then we can approximately obtain the self-energy:

$$\hat{\Sigma}(\phi,\omega) \approx \Bigg\{ \frac{4mT}{n_s(T)} \frac{1}{16\pi} \ln\left[\frac{\Lambda^2 + \tilde{\Delta}^2(\phi) + \tilde{\omega}^2}{\tilde{\Delta}^2(\phi) + \tilde{\omega}^2}\right]$$
$$+ \sum_\mathbf{q} \frac{T \ w^2(\phi)}{a + b \ q^2} \ \frac{1}{\tilde{\omega}^2 + (\mathbf{v}_F(\phi)\cdot\mathbf{q})^2 + \tilde{\Delta}^2(\phi)} \Bigg\}$$
$$\times \begin{pmatrix} -i\tilde{\omega} & \tilde{\Delta}(\phi) \\ \tilde{\Delta}(\phi) & -i\tilde{\omega} \end{pmatrix}, \quad (11)$$

where $\tilde{\omega}$ and $\tilde{\Delta}$ can be calculated self-consistently by $\hat{G}^{-1}(\phi;\mathbf{k},\omega) = \hat{G}_0^{-1}(\phi;\mathbf{k},\omega) - \hat{\Sigma}(\phi,\omega)$.

From the self-energy obtained in Eq. (11), by analytically continuing the frequency $i\omega \to \omega + i\eta$, we can calculate various single-particle properties such as density of states (DOS), spectral functions, and single-particle scattering rates. In this paper we focus on DOS since it is gauge-invariant and measurable via the tunneling spectroscopy[13] or the momentum-integrated ARPES data[14]. We are especially interested in the angle-resolved DOS:

$$N(\phi,\omega) = -\frac{1}{\pi}\mathrm{Im}\int d\xi_{\mathbf{k}}\ \mathrm{Tr}\ \hat{G}(\phi;\mathbf{k},\omega)\ , \tag{12}$$

as it gives information about the angular variation of the fluctuation effect.

Throughout this paper, we set the relevant energy scales $\Lambda \approx 10\Delta_0(T=0)/v_F$ and $E_F \approx 5\Lambda v_F$ so that we are well in the BCS weak-coupling regime; these relative energy scales give much stronger pairing strength than ordinary superconductors but significantly weaker than the cuprates. With the energy scales so chosen, we may estimate the regime of the validity of the mean-field theory. If we apply the Ginzburg criterion, namely, $|\Delta_0(T)|^2 \gg \langle d(\mathbf{x})\ d(\mathbf{x})\rangle$, which may be estimated from Eq. (7), the mean-field theory breaks down only near $T/T_c \sim 0.98$. Therefore, the BCS framework is reliable in most of the temperature range that we consider.

In Fig. 1 we show the total DOS. As the temperature increases, the DOS peak is widely smeared. Very close to T_c, the DOS peak has almost disappeared and the spectral gap is only manifested by the depletion in the DOS around $\omega = 0$ as compared to the normal state DOS. Figure 2 shows the DOS peak position as a function of temperature; in most of the temperature range, we can interpret the peak position roughly as the spectral gap. This figure shows that the spectral gap is reduced in a wide temperature range due to the order parameter fluctuations. Near $T/T_c \approx 0.98$, the DOS peak structure has almost disappeared, and the DOS maxima do not have a meaning as the spectral gap. Therefore, we need to estimate the size of the spectral gap from the width of the DOS depletion in this case. It is difficult to study the evolution of the spectral gap through T_c in this framework because the mean-field theory breaks down sufficiently close to T_c as discussed above. Also the result near zero temperature is not reliable due to the negligence of the time-dependence of the fluctuations.

The angle-dependent DOS peak near T_c is shown in Fig. 3. At $T \ll T_c$, the DOS peak contour follows the d-wave shape. As the temperature approaches T_c, we observe that the DOS is widely smeared to low-energy states especially near the antinode ($\phi = 0$). Figure 3 shows that the shape of the angle-resolved gap (DOS peak curve) is deformed from the original d-wave shape near the node. We argue that the downward bending of the DOS peak curve near the node ($\phi = \pi/4$) is due to the phase fluctuations since the amplitude fluctuations alone do not cause the downward bending as illustrated in the same figure. We find that the angle-dependence of the spectral gap near the node is

$$\begin{aligned}|\tilde{\Delta}(\phi)| \approx{}& \Delta_0(T)|\cos(2\phi)| \\ &\times\left\{1 - \frac{mT}{2\pi n_s(T)}\ln\left[\frac{\Lambda}{\Delta_0(T)|\cos(2\phi)|}\right]\right\}\ ,\end{aligned} \tag{13}$$

and the slope of the gap near the node is reduced. It has similarity to the shape of the gap obtained by ARPES on underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) in the superconducting state,[11] although its microscopic origin is not well understood.

Figure 4 shows angular variation of the scattering rate due to the order parameter fluctuation. We observe that the maximum scattering rate occurs near the antinode and also that the rate decreases as one approaches the node. This variation is due to the angular dependence of the order parameter magnitude fluctuations. This feature may contribute to the anisotropy of the quasiparticle scattering rate in cuprate superconductors.[14]

Discussions and Conclusions.—Here we discuss the qualitative effects of amplitude and phase fluctuations. In Fig. 3, we find that if we omit the phase fluctuation effect, the apparent gap is enhanced. This is because the amplitude fluctuations tend to increase the gap magnitude. This can be understood from the Fermi liquid reference frame as following: The fermion self-energy correction due to the amplitude fluctuations can be roughly estimated as

$$\begin{aligned}\Sigma(\mathbf{p},\omega) &\approx -\int d\nu d^2q G(\mathbf{p}-\mathbf{q},\omega-\nu)\ \langle\Delta(\mathbf{q},\nu)\Delta(-\mathbf{q},-\nu)\rangle \\ &\approx \frac{1}{i\omega+\xi_p}\langle\Delta(x)\Delta(x)\rangle\ ,\end{aligned} \tag{14}$$

and therefore the effective spectral gap is enhanced by the fluctuations as $|\Delta_{\text{eff}}|^2 = \langle\Delta(x)\Delta(x)\rangle = |\Delta_0|^2 + \langle\delta\Delta(x)\delta\Delta(x)\rangle$.

The effect of phase fluctuation can be considered as a Doppler shift in the fermionic spectrum by $\mathbf{k}_F \cdot \mathbf{v}_s$ where $\mathbf{v}_s \sim \nabla\theta/m$. Due to thermally fluctuating superfluid velocity, the DOS near the gap is now shifted since the energy levels at the gap nodes are enhanced. As a result, more states would be occupied near the nodes, and hence decrease in the slope of the gap nodes as shown in Fig. 3. On including the vortex pair unbinding transition of the BKT type, which gives stronger phase fluctuation effects, we can obtain a Fermi arc-like phenomenon.[6,15]

In order to obtain the correct effect on the size of the spectral gap, both the phase and amplitude fluctuations have to be self-consistently taken into account. The total effect is reduction in the spectral gap as shown in Fig. 2 and 3. However, the spectral gap may not be equal to the order parameter magnitude especially if the fluctuation is strong,[16] and hence more careful study is needed to separate these two quantities.

The results presented in this report are equally well applicable to any unconventional superconducting symmetry. In principle, any superconductor would have a

window of temperatures near T_c where such fluctuations are visible, depending on the pairing strength and the superfluid density. In case of underdoped cuprates, however, it would be essential to include the effect of vortex pair unbinding in the pseudogap state, due to the small superfluid density. The result of this report may nevertheless pertain to its superconducting state. Indeed, a recent observation of the deformed gap shape in Bi2212,[11] which is only observed in underdoped regime, may be related to the order parameter fluctuation effects, considering that the phase fluctuations are more important in underdoped cuprates due to reduced superfluid density. Since the microscopic origin of this deformation is not understood, further experimental investigation on the temperature variation of the gap anisotrpy would be desirable.

Some of the above features are shown to be shared by other theoretical results in the normal state counterpart. For instance, the form of the density of states obtained above is similar to that above T_c when the Gaussian pairing fluctuations are incorporated.[17] Also a similar but much more pronounced deformation of the d-wave spectral gap was obtained above T_c using a self-consistent conserving approximation.[18]

The author thanks Alan Dorsey and Rob Wickham for helpful discussions and comments. This work was supported by the National High Magnetic Field Laboratory and by NSF grant DMR 96-28926.

---

* Electronic mail: hjk@phys.ufl.edu.

[1] For an overview of the experimental results and their interpretation, see M. Randeria, cond-mat/9710223.

[2] See, for example, N. Miyakawa, *et al.*, cond-mat/9809398. See also Ref. [12].

[3] J. Maly, B. Janko, and K. Levin, Phys. Rev. B **59**, 1354 (1998); Y.-M. Vilk *et al*, J. Phys. Chem. Solids **59**, 1873 (1998); M. Capezzali and H. Beck, cond-mat/9806211, to appear in Physica B.

[4] See also the review article, A. A. Varlamov, G. Balestrino, E. Milani, and D. V. Livanov, to appear in Adv. Phys.

[5] V. J. Emery and S. A. Kivelson, Nature **374**, 434 (1995); J. Corson *et al.*, cond-mat/9810280.

[6] H.-J. Kwon and A. T. Dorsey, cond-mat/9809225 (Phys. Rev. B March 1999).

[7] J. R. Engelbrecht, M. Randeria, and C. A. R. Sa de Melo, Phys. Rev. B **55**, 15153 (1997).

[8] A. A. Varlamov and V. V. Dorin, Sov. JETP **64**, 1159 (1986).

[9] R. A. Smith, M. Yu. Reizer, and J. W. Wilkins, Phys. Rev. B **51**, 6470 (1995).

[10] M. R. Norman *et al.*, Nature **392**, 157 (1998).

[11] J. Mesot, *et al.*, cond-mat/9812377.

[12] A. G. Aslamazov and A. I. Larkin, Soviet Solid State, **10**, 875 (1968).

[13] Ch. Renner *et al.*, Phys. Rev. Lett. **80**, 149 (1998); A. K. Gupta and K.-W. Ng, Phys. Rev. B **58**, R8901 (1998).

[14] D. S. Marshall *et al.*, Phys. Rev. Lett. **76**, 4841 (1996); H. Ding *et al.*, Nature **382**, 51 (1996); M. R. Norman, M. Randeria, H. Ding and J. C. Campuzano, Phys. Rev. B **57**, R11093 (1998); H. Ding *et al.*, cond-mat/9712100.

[15] M. Franz and A.J. Millis, Phys. Rev. B **58**, 14572 (1998).

[16] I. Kosztin, Q. Chen, B. Janko, and K. Levin, Phys. Rev. B **58**, R5936 (1998).

[17] S. Marcelja, Phys. Rev. B **1**, 2351 (1970).

[18] J. R. Engelbrecht, A. Nazarenko, M. Randeria, and E. Dagotto, Phys. Rev. B **57**, 13406 (1998).

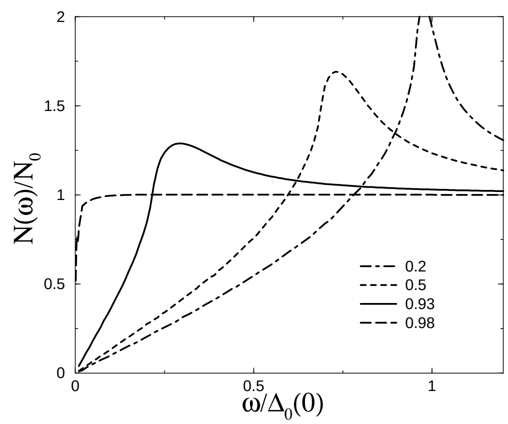

FIG. 1. Total density of states ($N(\omega)/N_0$) as a function of energy at four temperatures (T/T_c = 0.2, 0.5, 0.93, and 0.98).

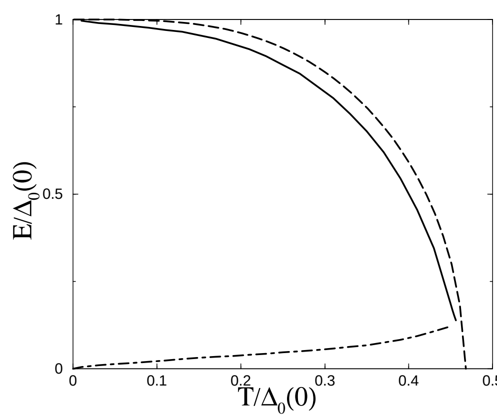

FIG. 2. The comparison of the density of states peak to the mean-field gap magnitude. The solid line is the total density of states peak position and the long dashed line is the mean-field gap. The dot-dashed line is the difference between the two quantities.

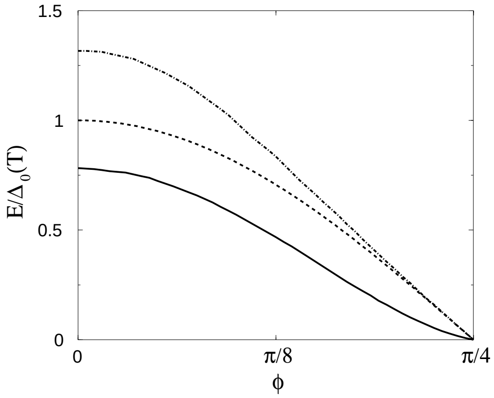

FIG. 3. The peak points of the angle-resolved density of states (solid line) vs the mean-field gap (dashed line) at $T/T_c = 0.93$. The dot-dashed line is the DOS peak curve evaluated with only the order parameter amplitude fluctuations.

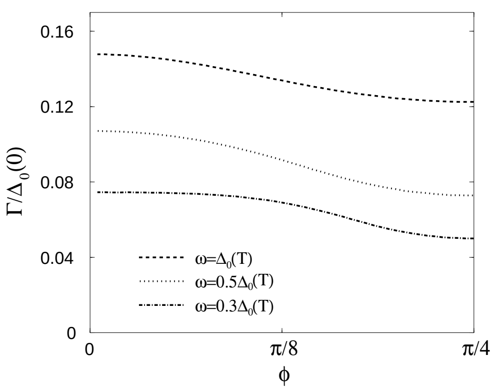

FIG. 4. The angular variation of the quasiparticle scattering rate ($\Gamma(\omega)/\Delta_0(0)$) evaluated at $\omega/\Delta_0(T) = 1,\ 0.5$, and 0.3 at $T/T_c = 0.93$.